Supporting Information for

Structure and water attachment rates of ice in the atmosphere: role of nitrogen

by

P. Llombart, R. Bergua, E. G. Noya and L. G. MacDowell

Instituto de Química Física Rocasolano , CSIC, Calle Serrano 119, 28006 Madrid, Spain

and

Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense, Madrid, 28040, Spain.

ρ	T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ	T	P
	230	0.39		230	0.55		230	0.71		230	0.87		230	1.01		230	1.14		230	1.25
	235	0.40		235	0.55		235	0.70		235	0.88		235	0.99		235	1.17		235	1.35
	240	0.39		240	0.57		240	0.72		240	0.88		240	1.08		240	1.24		240	1.37
	245	0.42		245	0.59		245	0.74		245	0.91		245	1.08		245	1.25		245	1.42
0.56	250	0.42	0.79	250	0.58	1.03	250	0.75	1.26	250	0.94	1.50	250	1.11	1.73	250	1.29	1.96	250	1.42
	255	0.42		255	0.59		255	0.78		255	0.94		255	1.09		255	1.29		255	1.45
	260	0.43		260	0.60		260	0.80		260	0.95		260	1.16		260	1.34		260	1.48
	265	0.44		265	0.62		265	0.80		265	1.00		265	1.11		265	1.33		265	1.52
	270	0.46		270	0.64		270	0.82		270	1.02		270	1.19		270	1.39		270	1.55

TABLE I: Equation of State for nitrogen. Pressure (P) is expressed in units of 10^5 Pa, temperature (T) in K and density (ρ) in kg m^{-3}.

T	$B_2(T)$
K	$10^3\ kg^{-1}m^3$
270	-3.2
265	-11.9
260	-5.9
255	-13.8
250	-4.5*
245	-3.4*
240	-4.7*
235	-13.0
230	-20.9

TABLE II: Effective second virial coefficient B_2 as a function of temperature. * Three out layers were not included in the fit for $B_2(T)$.

$Face$	T	Lx	Ly	Lz	Number of N_2	$\rho_{N_2}^{bulk}$
	K	nm	nm	nm		kgm^{-3}
Basal	270	7.26698	6.29362	15.00000	0	0
				36.85765	46, 44, 42, 37, 32	0.95, 1.10, 1.24, 1.31, 1.37
	260	7.26350	6.29060	15.00000	0	0
				36.85765	49, 46, 43, 36, 29	0.86, 1.06, 1.27, 1.36, 1.46
	250	7.25949	6.28713	15.00000	0	0
				36.85765	53, 50, 47, 30, 25	0.74, 0.89, 1.40, 1.48, 1.56
	240	7.25609	6.28412	15.00000	0	0
				36.88880	48, 45, 37, 21	0.62, 1.09, 1.33, 1.41
	230	7.25229	6.28104	15.00000	0	0
				36.58888	50, 33, 17	0.50, 0.98 1.48
pI	270	7.26707	5.91452	15.00000	0	0
				36.85765	46, 44, 42, 37, 32	1.02, 1.18, 1.34, 1.40, 1.46
	260	7.26329	5.91143	15.00000	0	0
				36.85765	49, 46, 43, 36, 29	0.92, 1.15, 1.37, 1.46, 1.55
	250	7.25957	5.90841	15.00000	0	0
				36.85765	53, 50, 47, 30, 25	0.79, 0.95, 1.42, 1.52, 1.58
	240	7.25604	5.90554	15.00000	0	0
				35.58888	48, 45, 37, 21	0.69, 1.22, 1.48, 1.58
	230	7.25229	5.90249	15.00000	0	0
				35.85765	50, 33, 17	0.55, 1.07, 1.62

TABLE III: Summary of thermodynamic conditions and system sizes for the simulations of the ice interface in presence of nitrogen.

$Facet$	T / K	N_{N_2}	N_{ns}	N_{ev}	α
Basal	270	42	14 (14)	2	0.9650
Basal	270	0	0	0	1.0000
Basal	260	43	12 (9)	2	0.9700
Basal	260	0	6	1	0.9850
Basal	230	50	14 (11)	0	0.9650
Basal	230	0	5	0	0.9875
pI	270	42	13 (10)	2	0.9675
pI	270	0	1	1	0.9975
pI	260	43	13 (11)	2	0.9675
pI	260	0	1	0	0.9975
pI	230	50	20 (19)	0	0.9500
pI	230	0	0	0	1.0000

TABLE IV: Table with detailed information of the collision statistics. N_{N_2} is the number of nitrogen molecules present in the simulation box. N_{ns} is the number of water molecules shot a distance of 2 nm away from the surface and not sticking into the surface. Shown in parenthesis is the number of molecules which were reflected back to the gas phase by collisions with nitrogen gas molecules. N_{ev} provides the number of evaporation events observed during the simulations.

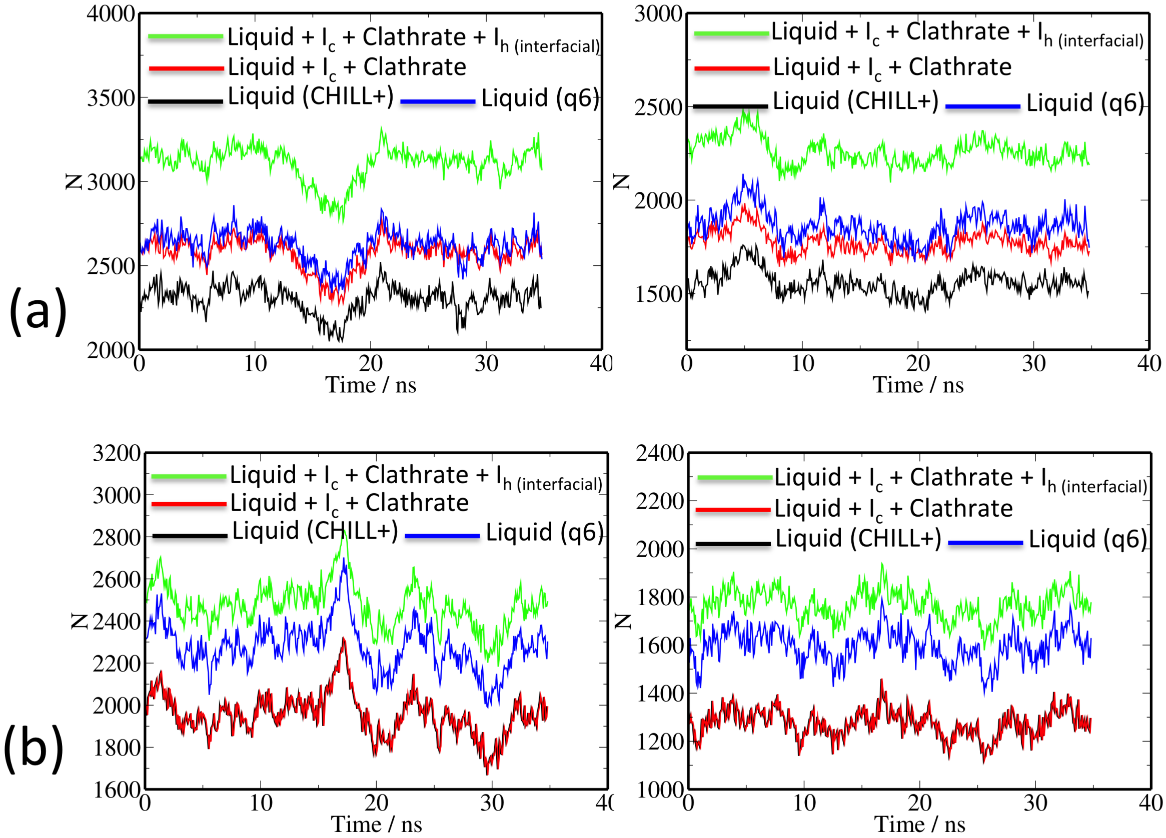

FIG. 1: Comparison of the number of liquid-like molecules as determined from the $\bar{q}_6$ parameter and the CHILL+ algorithm.[84]. a) Results for the Basal plane. b) Results for the prismatic plane. Plots are shown from left to right at 270, 260, 250, 240 and 230 K, respectively. Blue: Runing number of liquid molecules during a simulation as obtained from the $\bar{q}_6$ parameter used in this work. Black: Runing number of liquid molecules as a function of time as extracted with the CHILL+ algorithm. Notice that the blue and black lines run almost parallel to each other, with a constant offset of about 12%. Other possible choices to determine the thickness of the premelting layer remain also largely correlated. Red: Runing number of molecules in liquid, cubic and clathrate like environments as obtained from the CHILL+ algorithm. Green: Running number of molecules in liquid, cubic, clathrate, and interfacial hexagonal environments as obtained from the CHILL+ algorithm.

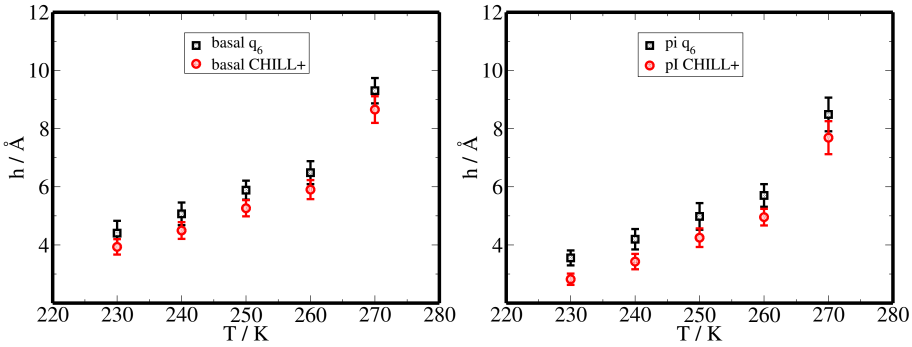

FIG. 2: Left: Basal. Right: pI. Premelting thickness at zero nitrogen pressure as calculated using the number of liquid like molecules from $\bar{q}_6$ (squares) used in this work and the CHILL+ algorithm (circles). Notice that the calculation of film heights differs by an almost constant offset.